

Collective modes in unconventional density waves

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Abstract. – We have investigated the collective modes of unconventional charge and spin density waves (UCDW, USDW) in quasi-one dimensional systems in random phase approximation. The density correlator regains its normal state form due to the phase degree of freedom of the condensate. The possible effect of impurities is also discussed. From this, the current-current correlation function is evaluated through charge conservation. The spin susceptibility of USDW remains anisotropic in spite of the lack of any periodic modulation of the spin density. In UCDW, the spin response gets weaker in all three directions as the temperature is lowered.

Unconventional density waves were intensively studied over the past few years. The so called d-density wave, which is UCDW with a gap of $d_{x^2-y^2}$ symmetry, has attracted much attention [1]. This model successfully described many aspects of the pseudogap phase of high temperature cuprate superconductors. Also d-wave SDW can account for the anomalously small magnetic ordering in URu₂Si₂ [2, 3]. In quasi-one dimensional systems, our UCDW model describes successfully the behaviour of the low temperature phase of α -(BEDT-TTF)₂KHg(SCN)₄ [4, 5, 6], including the angular dependent magnetoresistance [7]. The response of (TMTSF)₂PF₆ for $T < T^* \sim 4\text{K}$ can be described if the creation of USDW is assumed on top of the existing SDW [8].

The effect of collective modes is very important to study the dynamics of a system. The pole structure of the susceptibility is of prime importance [9, 10, 11]: at a given combination of the wavevector and frequency, the response function can be divergent. This means, that even without external field, excitations occur in the system whose dispersion is determined by the poles of the susceptibility. One way of identifying the correct order parameter among possible candidates is to study the unique collective modes supported by the ground state of a given symmetry [12, 13, 14, 15, 16], as it was done in unconventional superconductors.

Allowing for a low temperature phase transition, the Green's function of the model changes and new type of anomalous Green's functions can enter (for example the Gor'kov type $F(i\omega_n, \mathbf{k})$ function belonging to the $\langle a_{\mathbf{k},\downarrow}^+ a_{-\mathbf{k},\uparrow}^+ \rangle$ pair correlation in superconductivity). Consequently new types of interaction channels might open due to the novel type of nonvanishing expectation value, which is called the fluctuation of the order parameter [9, 10]. As a result, the

simple RPA series is modified, and a number of coupled geometrical series are to be summed up. In the case of a conventional DW, the collective modes are well-known [17,18,19,20,21,22]. Generally one can conjecture whether the effect of RPA is or is not to re-establish the original pole structure of the metallic state. This can be achieved due to the degree of freedom of the phase of the density wave or the direction of the spin polarization of SDW. If we face with a magnetic phase transition (with a given spin orientation, i.e. SDW), the transverse (to the preferred direction) spin susceptibility and the density correlation function are not relevant from the transition's point of view, hence they will be restored. The former does due to the low energy (gapless) excitations of the spins in the perpendicular directions while the latter due to the free phase. Similarly the density correlator would regain its original form after RPA in a CDW due to the unrestricted phase of the density wave, but through the phonon mediated interaction the collective contribution is modified because of the mass enhancement. The quantities which are expected to change are the longitudinal spin susceptibility in SDW and all the spin susceptibilities in CDW because there are no low energy excitations based on the degrees of freedom of the system.

From now on, we introduce the formalism necessary to investigate the collective modes in RPA and evaluate possible excitations of the main quantities.

Formalism for RPA. – To start with, it is useful to introduce the spinor, which covers the whole momentum-spin space:

$$\Psi(\mathbf{k}, \tau) = \begin{pmatrix} a_{\mathbf{k},\uparrow}(\tau) \\ a_{\mathbf{k}-\mathbf{Q},\uparrow} \\ a_{\mathbf{k},\downarrow}(\tau) \\ a_{\mathbf{k}-\mathbf{Q},\downarrow} \end{pmatrix}, \quad (1)$$

where $a_{\mathbf{k},\sigma}$ is the annihilation operator of an electron of momentum \mathbf{k} and spin σ , \mathbf{Q} is the best nesting vector. From this the Green's function of USDW is obtained as

$$G(\mathbf{k}, i\omega_n) = -\frac{i\omega_n + \xi(\mathbf{k})\rho_3 + \Delta(\mathbf{k})\rho_1\sigma_3}{\omega_n^2 + \xi(\mathbf{k})^2 + \Delta(\mathbf{k})^2}, \quad (2)$$

for UCDW σ_3 has to be replaced with 1, where σ_i ($i = 1, 2, 3$) are the Pauli matrices acting on spin space. With this, the interaction responsible for the UDW formation is determined from the gap equation of Ref. [23] and assuming $\Delta(\mathbf{k}) = \Delta \sin(bk_y)$ without loss of generality, it is given by

$$\begin{aligned} \frac{N}{V} \tilde{V}(\mathbf{k}, \mathbf{k}', \mathbf{q}, \sigma, \sigma') &= \delta_{-\sigma, \sigma'} (2J_y \sin(bk_y) \sin(b(k'_y - q_y)) - \\ &- 2F_y \sin(bk_y) \sin(bk'_y)) + \delta_{\sigma, \sigma'} (J_y - V_y) \sin(bk_y) \sin(b(k'_y - q_y)), \end{aligned} \quad (3)$$

Of course the interaction is able to support $\Delta \cos(bk_y)$ type of gap, but we neglected the terms favouring this specific wavevector dependence: they are irrelevant with respect to RPA because they can only renormalize the coefficients of the susceptibilities but are unable to drive the system into the desired ground state, namely with sinusoidal gap. This approximation was used in the first step of the calculation, namely in the gap equation [23], when the specific wavevector dependence of the gap was chosen, because the matrix elements favouring this ordering are assumed to be the strongest. All the following calculations apply also to a cosinusoidal gap. For simplicity we shall limit our analysis to $\mathbf{q} = (q_x, 0, 0)$ (i.e. wavevector pointing in the quasi-one dimensional direction).

Density correlator and complex conductivity. – For the density-density correlator we obtain for UDW

$$\langle [n, n] \rangle = \langle [n, n] \rangle_0 + \frac{P_i}{4} \langle [n, A_i] \rangle_0 \langle [A_i, n] \rangle, \quad (4)$$

$$\langle [A_i, n] \rangle = \langle [A_i, n] \rangle_0 + \frac{P_i}{4} \langle [A_i, A_i] \rangle_0 \langle [A_i, n] \rangle, \quad (5)$$

where $\langle \dots \rangle_0$ means the thermal average without interaction between fluctuations. Here $i = c, s$ for UCDW and USDW, respectively. $A_s = \rho_2 \sigma_3 \sin(bk_y)$, $A_c = \rho_2 \sin(bk_y)$ and both P_c and P_s are positive. The detailed form of the interaction (P) can be found in Ref. [23]. The retarded products $\langle [n, n] \rangle_0$, etc. are evaluated within the standard method and we find

$$\langle [n, n] \rangle_0 = 2g(0) \frac{\xi^2}{\xi^2 - \omega^2} (1 - 4\Delta^2 F), \quad (6a)$$

$$\langle [n, A_i] \rangle_0 = -i4g(0)\xi\Delta F, \quad (6b)$$

$$\langle [A_i, A_i] \rangle_0 = 2g(0) \left(\frac{2}{P_i g(0)} + (\omega^2 - \xi^2) F \right), \quad (6c)$$

where $g(0)$ is the density of states at the Fermi energy in the normal state per spin, $\xi = v_F q_x$, $\langle [n, n] \rangle_0(\mathbf{q}, \omega)$ is obtained, for example, after analytic continuation from

$$\langle [n, n] \rangle_0(\mathbf{q}, i\omega_\nu) = -\frac{1}{\beta V} \sum_{\mathbf{k}, n} \text{Tr}(G(\mathbf{k}, i\omega_n) G(\mathbf{k} - \mathbf{q}, i\omega_{n-\nu})) \quad (7)$$

and

$$F = (\xi^2 - \omega^2) \frac{1}{2\pi} \int_0^\infty \int_0^{2\pi} \tanh \frac{\beta E}{2} \frac{N}{D} \text{Re} \frac{\sin(y)^2}{\sqrt{E^2 - \Delta^2 \sin(y)^2}} dy dE, \quad (8)$$

$$N = (\xi^2 - \omega^2)^2 - 4E^2(\xi^2 + \omega^2) + 4\Delta^2 \sin(y)^2 \xi^2, \quad (9)$$

$$D = N^2 - 64E^2 \omega^2 \xi^2 (E^2 - \Delta^2 \sin(y)^2), \quad (10)$$

is the F function which also appears in the correlation functions of conventional DW with constant gap [20]. The extra $\sin(y)^2$ factor in the numerator of the density of states like term comes either from the gap or from the interaction. The remaining angle integral (which is the Fermi surface average) can be performed and after straightforward manipulation it yields to

$$\begin{aligned} 4\Delta^2 F = & \frac{\xi^2 - \omega^2}{\xi^2} \frac{2}{\pi} \left\{ \int_0^\Delta dE \tanh \frac{\beta E}{2} \left[\frac{N_1}{2\Delta D_1} \Pi \left(-\frac{4\xi^2 E^2}{D_1}, \frac{E}{\Delta} \right) + \frac{1}{\Delta} K \left(\frac{E}{\Delta} \right) + \right. \right. \\ & \left. \left. + \frac{N_2}{2\Delta D_2} \Pi \left(-\frac{4\xi^2 E^2}{D_2}, \frac{E}{\Delta} \right) \right] + \right. \\ & \left. + \int_\Delta^\infty dE \tanh \frac{\beta E}{2} \left[\frac{N_1}{2ED_1} \Pi \left(-\frac{4\xi^2 \Delta^2}{D_1}, \frac{\Delta}{E} \right) + \frac{1}{E} K \left(\frac{\Delta}{E} \right) + \frac{N_2}{2ED_2} \Pi \left(-\frac{4\xi^2 \Delta^2}{D_2}, \frac{\Delta}{E} \right) \right] \right\}, \end{aligned} \quad (11)$$

where $K(z)$ and $\Pi(n, z)$ are the complete elliptic integral of the first and third kind [24], respectively and

$$N_1 = (-E^2 - \xi^2 + (E - \omega)^2)(\xi^2 - (2E - \omega)^2), \quad (12a)$$

$$D_1 = (E^2 + \xi^2 - (E - \omega)^2)^2 - 4\xi^2 E^2, \quad (12b)$$

$$N_2 = (-E^2 - \xi^2 + (E + \omega)^2)(\xi^2 - (2E + \omega)^2), \quad (12c)$$

$$D_2 = (E^2 + \xi^2 - (E + \omega)^2)^2 - 4\xi^2 E^2. \quad (12d)$$

Putting these expressions together we obtain

$$\langle [n, n] \rangle(\omega, q) = 2g(0) \frac{\xi^2}{\xi^2 - \omega^2}, \quad (13)$$

which is the same as in the normal state. It is worth mentioning that in conventional SDW the coefficient of ξ^2 in the denominator is $1 + Ug(o)$ [20], U is the on-site Coulomb repulsion. The strength of interaction is missing here due to its zero average over the Fermi surface (See Eq. (3)). In the absence of the DW pinning, all the modifications due to the change of quasiparticle spectrum are exactly canceled from the contribution of the fluctuation of the order parameter. The coupled RPA equations consist of two parts: the single particle contribution (one bubble contribution) which arises from the thermal excitation across the gap and possibly from a remnant portion of the Fermi surface, and the collective part from the motion of the density wave as a whole (due to the freedom of the phase) [25]. In the case of $\langle [n, n] \rangle$, these two cancel each other to give back the normal state form.

In real systems, impurities are always present. Henceforth the easiest way to incorporate the effect of impurities is to modify Eq. (6c) as in Ref [20] as

$$\langle [A_i, A_i] \rangle_0 = 2g(0) \left(\frac{2}{P_i g(0)} - (\xi^2 + \omega_p^2 - \omega^2) F \right), \quad (14)$$

where ω_p is the pinning frequency. This is the zeroth order phason propagator, and the inclusion of ω_p ensures the presence of gapped phason mode. In general, impurities act differently on UDW [26] than on conventional DW, but extended impurities are able to pin the phase of UDW, inducing finite pinning frequency [4]. As a result, the density correlator reads as

$$\langle [n, n] \rangle(\omega, q) = 2g(0) \xi^2 \frac{\xi^2 - \omega^2 + \omega_p^2(1 - f)}{(\xi^2 - \omega^2)(\xi^2 + \omega_p^2 - \omega^2)} \quad (15)$$

for both USDW and UCDW, $f = 4\Delta^2 F$. The zero sound dispersion ($\omega^2 = \xi^2$) cancels out here contrary to the conventional case [20], because a detailed study of the f function reveals that $f = 1 + \text{const}(\xi^2 - \omega^2)/\Delta^2$ in the limit of ω tends to ξ . The pole of the propagator describes the pinned dynamics of the USDW and UCDW condensate as $\omega^2 = \omega_p^2 + \xi^2$. Due to pinning, the condensate does not move below the threshold frequency ω_p . The sound velocity in the presence of the electron-phonon coupling (g_{e-ph}) is given by

$$C = C_0 \sqrt{1 - g_{e-ph}^2 \lim_{q \rightarrow 0} \langle [n, n] \rangle(0, q)}, \quad (16)$$

where C_0 is the sound velocity without the electron-phonon coupling. First, in the absence of the DW pinning the sound velocity is temperature independent and reads as

$$C = C_0 \sqrt{1 - \lambda} \quad (17)$$

with $\lambda = 2g_{e-ph}^2 g(0)$. Second, in the presence of pinning we obtain for UDW

$$C = C_0 \sqrt{1 - \lambda(1 - \rho_s)}, \quad (18)$$

where ρ_s is the static condensate density [23], $\rho_s = \lim_{q \rightarrow 0} \lim_{\omega \rightarrow 0} f$. Since ρ_s increases as the temperature decreases, we predict increasing sound velocity by lowering the temperature below its critical value T_c for both UDW system.

From the density correlator the complex conductivity in the chain direction is obtained using charge conservation as

$$\sigma(\omega, q) = 2g(0)ie^2\omega \frac{\omega^2 - \omega_p^2(1 - f) - \xi^2}{(\xi^2 - \omega^2)(\xi^2 + \omega_p^2 - \omega^2)}. \quad (19)$$

From this the optical conductivity of UDW reads as $\text{Re}\sigma(\omega) = 2g(0)e^2\pi\delta(\omega)$ in the pure case, which is essentially the same formula as in the normal state. Note that this formula applies for UCDW because there is no mass renormalization associated with lattice distortion. If conventional CDW is deduced from the attractive Hubbard model [25, 19], its conductivity coincides with those of a conventional SDW (using a phonon mediated attractive interaction, the mass gets renormalized in CDW). In the $q \rightarrow 0$ limit the conductivity is the same as in conventional SDW, only the f function should be replaced by its version corresponding to UDW:

$$\sigma(\omega, 0) = 2g(0)\frac{e^2}{i\omega} \left(f_0 - 1 - \frac{f_0\omega^2}{\omega^2 - \omega_p^2} \right) \quad (20)$$

with $f_0 = 4\Delta^2 F_{q=0}$. It approaches the one in the normal state for $\omega \gg \omega_p$ for USDW and UCDW, while this statement is not true in CDW because $m^*/m \gg 1$. The peak at zero frequency in the optical conductivity moves to the pinning frequency, suggesting that the primitive mimicking of pinning was successful.

The conductivity for electric field applied in the z direction remains unchanged because the interaction is unable to dress the single bubble contribution due to the wavevector dependence of the velocity. In the y direction where the gap is developed, the following equation is to be solved:

$$\langle [j_y, j_y] \rangle = \langle [j_y, j_y] \rangle_0 - \frac{P_j}{4e^2 v_y^2} \langle [j_y, j_y] \rangle_0 \langle [j_y, j_y] \rangle, \quad (21)$$

where $P_j = -P_c$, the matrix element responsible for the UCDW instability, and the current correlator without interaction between fluctuations is obtained as

$$\langle [j_y, j_y] \rangle_0(\omega, q) = 4e^2 v_y^2 g(0) \frac{1}{\xi^2 - \omega^2} (\xi^2 - \omega^2 f), \quad (22)$$

which gives the paramagnetic part of the total conductivity. Here the explicit wavevector dependence of the gap plays an important role. If the system possess a gap with cosine, the interaction is unable to dress the one bubble diagram, hence it gives the total paramagnetic part. The RPA equation is true only for a gap $\sim \sin(bk_y)$. Adding the diamagnetic term to it, the complex conductivity reads as

$$\sigma_{yy} = \frac{\sigma_{yy0} - \frac{g(0)P_j}{2}(\sigma_{yy0} - \sigma_n)}{1 - \frac{g(0)P_j}{2} \left(\frac{\sigma_{yy0}}{\sigma_n} - 1 \right)}, \quad (23)$$

where $\sigma_n = -2g(0)e^2v_y^2/i\omega$ is the normal state conductivity, σ_{yy0} is the conductivity without RPA. Only Fermi liquid type corrections are present. Hence the excitation spectrum in the y direction is given by $\omega^2 = (1 + g(0)P_j(1 - f_0))\xi^2$. This is very similar to the zero sound dispersion in the x direction in conventional SDW in the presence of pinning [20]. The sign of P_j is negative for UCDW but for USDW it can be positive as well. These calculations verify our earlier assumption in Ref. [23], that the optical conductivity in the perpendicular direction is given by the quasiparticle contribution, only Fermi liquid renormalization may occur.

Spin susceptibilities. – As to the spin susceptibility, the transverse one in USDW is expected to return to its normal state form similarly to the conventional case and to exhibit the trivial Goldstone mode. The RPA equations read as

$$\langle[\sigma_1, \sigma_1]\rangle = \langle[\sigma_1, \sigma_1]\rangle_0 + \frac{P}{4}\langle[\sigma_1, \rho_1\sigma_1]\rangle_0\langle[\rho_1\sigma_1, \sigma_1]\rangle, \quad (24)$$

$$\langle[\rho_1\sigma_1, \sigma_1]\rangle = \langle[\rho_1\sigma_1, \sigma_1]\rangle_0 + \frac{P}{4}\langle[\rho_1\sigma_1, \rho_1\sigma_1]\rangle_0\langle[\rho_1\sigma_1, \sigma_1]\rangle, \quad (25)$$

where

$$\langle[\sigma_1, \sigma_1]\rangle_0 = \frac{2g(0)}{\xi^2 - \omega^2}(\xi^2 - 4\Delta^2\omega^2F), \quad (26)$$

$$\langle[\sigma_1, \rho_1\sigma_1]\rangle_0 = 4g(0)i\Delta\omega F, \quad (27)$$

$$\langle[\rho_1\sigma_1, \rho_1\sigma_1]\rangle_0 = 2g(0)\left(\frac{2}{g(0)P} + (\omega^2 - \xi^2)F\right). \quad (28)$$

Putting these together we obtain

$$\langle[\sigma_1, \sigma_1]\rangle = 2g(0)\frac{\xi^2}{\xi^2 - \omega^2}. \quad (29)$$

In the static limit, this expression reduces to the well known Pauli susceptibility. The longitudinal susceptibility of USDW shows only Fermi liquid type renormalization, hence it is given mainly by the one bubble contribution, which coincides with the expression found for $\langle[n, n]\rangle_0(\mathbf{q}, i\omega_\nu)$ in Eq. (7). For UCDW the spin response is described with this expression in either direction. Although there is no obvious magnetic long range order in USDW [23], yet it retains the spin anisotropy of SDW: in the static, long wavelength limit the longitudinal susceptibility reads as $\langle[\sigma_3, \sigma_3]\rangle = 1 - \rho_s$, which vanishes as T goes to zero. The pole belonging to the usual spin wave dispersion $\omega^2 = \xi^2$ cancels out similarly to the case of the density correlator in the presence of pinning.

Conclusion. – We have studied the relevant correlation functions with random phase approximation. Again as in superfluid ^3He [9,10], the quantity whose correlator is investigated, often couples to the fluctuation of the UDW order parameter and it is necessary to handle these fluctuations on equal footing. Due to the unrestricted phase of the density wave, the density correlator regains its simple normal state form as it does in conventional spin density waves. In UCDW, the phason mass remains unrenormalized because the interaction from which this phase is originated, is electron-electron interaction and there are no retardation effects associated with electron-phonon interaction [22,19]. Based on a very simple concept [20] the pinning of UDW is incorporated into the theory and the sound velocity C is examined in the presence and absence of the pinning. Without pinning C does not change compared to the

normal state value. In a pinned UDW the sound velocity increases upon entrance in UDW. Additionally the conductivity in the chain direction is obtained from the density correlator through charge conservation. It does neither change compared to the one in the normal state: in the pure system $\text{Re}\sigma(\omega) \sim \delta(\omega)$, which inspired the first pioneers in this field to identify the origin of the mechanism leading to superconductivity as CDW formation.

By evaluating the current-current correlation function in the perpendicular directions, our previous assumption in Ref. [23] is verified: collective contributions do not show up and the quasiparticle contribution is enough to describe the electromagnetic response of the UDW.

The spin susceptibility of USDW shows antiferromagnetic like anisotropy [27, 28] in spite of the lack of magnetic ordering, while in UCDW the magnetic response is influenced mainly by the quasiparticle contribution, leading to the freezing out of the static susceptibilities at low temperatures in all directions, as we predicted in Ref. [23].

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